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13. ABSTRACT *(Maximum 200 words)*

The research effort addresses several issues related to non- linear transport in quantum wire systems characterized by spatially non-uniform confinement. We have successively investigated quantum transport through a variety of quantum cavities by using a Recursive Green Function Technique with emphasis on the effect of disorder on the conductance of the structure, one-dimensional transport in coupled quantum boxes structures with emphasis on the effect of suppression of optic phonon scattering on the transport properties, and finally the detailed influence of confined optic phonon modes on the scattering processes in quantum wires.

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TRANSPORT SIMULATION IN SPATIALLY MODULAED LOW-DIMENSIONALITY SYSTEMS

FINAL REPORT

J. P. LEBURTON

April 1, 1991 - September 30, 1994

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II. RESULTS OF RESEARCH UNDER PREVIOUS ARO GRANT

Research on "Transport Simulation in Spatially Modulated Low Dimensionality Systems," by J. P. Leburton is funded by ARO Grant No. DAAL03-91-G0052, from April 1, 1991 to September 30, 1994.

Research has focused on three areas: 1) modeling of transport in quantum cavity, 2) transport simulation of periodically modulated quantum wires, and 3) confined phonon scattering in quantum wires.

This research has resulted in 11 publications and 7 presentations at Symposia and Conferences. In addition, we have organized a NATO Advanced Research Workshop, supported by the European Research Office (ERO) of the US Army on "Phonons in Semiconductor Nanostructures" with J. Pascual and C. Sotomayor-Torres, in San Feliu de Guixols, Barcelona, Spain, September 1992.

II.1 Modeling of Transport through Quantum Cavity

We have thoroughly investigated quantum transport through a variety of double bend (DB) electron waveguide structures using the recursive Green's function techniques, and calculated the conductance using the two-probe multi-channel Landauer-Büttiker formula. We specifically focused on the influence of geometry, impurity scattering, interface roughness and finite temperature on the quantum conduction [P.7]. We found that the roundness of the corners washes out the resonance structures by increasing the conductance between the peaks. As expected from experimental results, impurity scattering and interface roughness slightly shift the resonance peak position and decrease their amplitudes which is in good agreement with the data of Wu et al. (SPIE Proceedings 1676 102 (1991)) (Fig.1.). Thermal averaging of the conductance leads to a decrease and broadening of the resonance peaks. For multiple double bend structures in series, we demonstrated the existence of an energy gap between the first and second subband threshold energies where the conductance is suppressed [P.6].

We have also conducted an experiment on conductance in DB structures with our colleagues of the Microelectronic Centers at the University of Illinois who demonstrated the onset of conductance oscillations up to 7K [P.10]. Our simulation indicates that these oscillations can not be accounted for by resonant tunneling via quasi-bound states below the first threshold energy in the lead because the tunneling barrier is too thick. Investigation is still underway to identify the cause of these oscillations at such a high temperature.

We have also investigated lateral tunneling of electrons through a one-dimensional (1D) double quantum well system with the Green's function technique [P.9]. We showed that a strong resonance manifests at the onset of conductance, and a "beating" effect due to competing characteristic times between tunneling and well propagation in the quantum well. We also showed that the finite conductance at large Fermi energies where the density of states for individual well is small can be exploited as a new principle for quantum interference transistor.

II.2 Transport Simulation in Periodically Modulated Quantum Wires

We have also investigated transport in 1D coupled quantum box (1D-CQB) structures at room temperature by using an iterative technique for solving the time-dependent Boltzmann Equation [P.4,P.5]. The scattering rates in the mini-Brillouin zone are characterized by several large peaks reflecting the singularities in the 1D density-of-states and the features of the miniband structure. As a result of Bragg refraction, the momentum distribution function deviates significantly from a displaced Maxwellian, with carrier accumulation at the miniband edges. Under suppression of optic phonon scattering, the time evolution of the distribution function, and the electron velocity under high electric field undergo damped

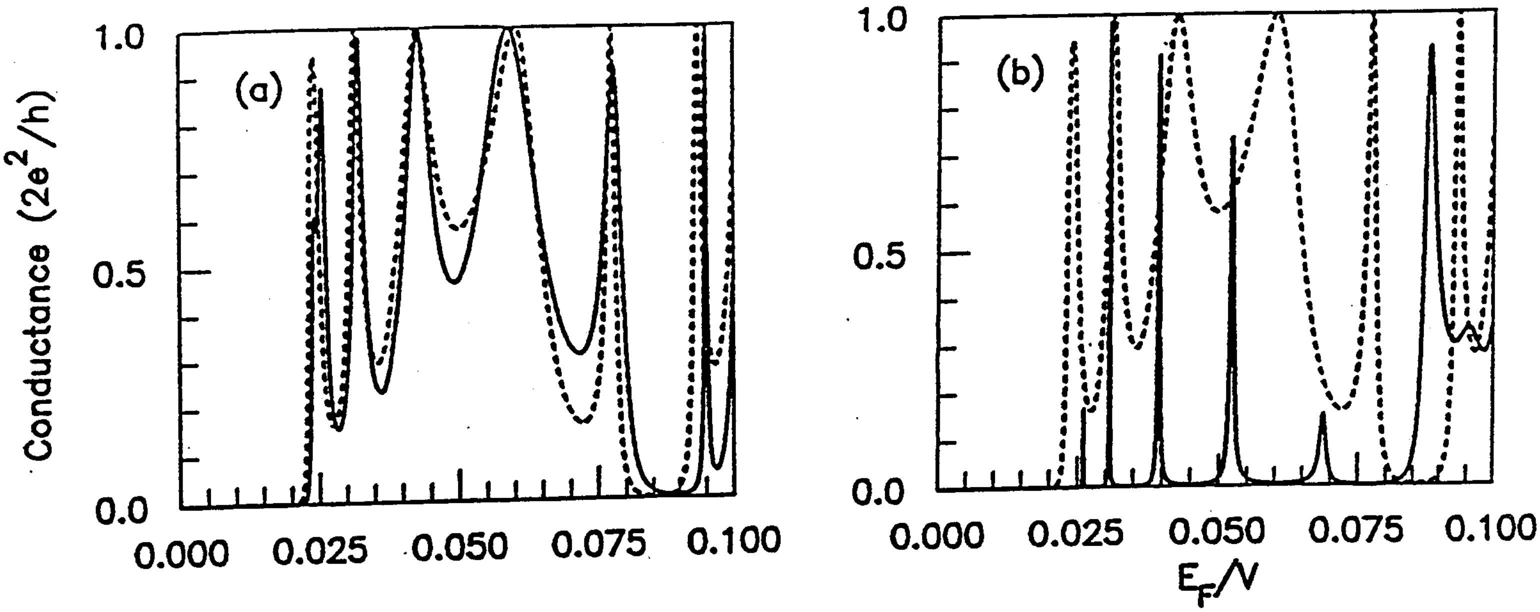

Fig. 1. The conductance G in units of $2e^2/h$ vs electron energy for the DB structure attached to a wide 2D region, for different degrees of disorder. A random value δ is added to each site energy $\varepsilon_{ij} + \delta$, where $|\delta| \leq \Delta/2$: (a) $\delta = 0.1$, and (b) δ=0.5. The conductance of the ideal structure without any impurities is given by the dotted lines. The energy is given in units of the hopping matrix element $V = \hbar^2/2m^* a^2$, where a is the lattice constant of the discretization. (After ref. P 7)

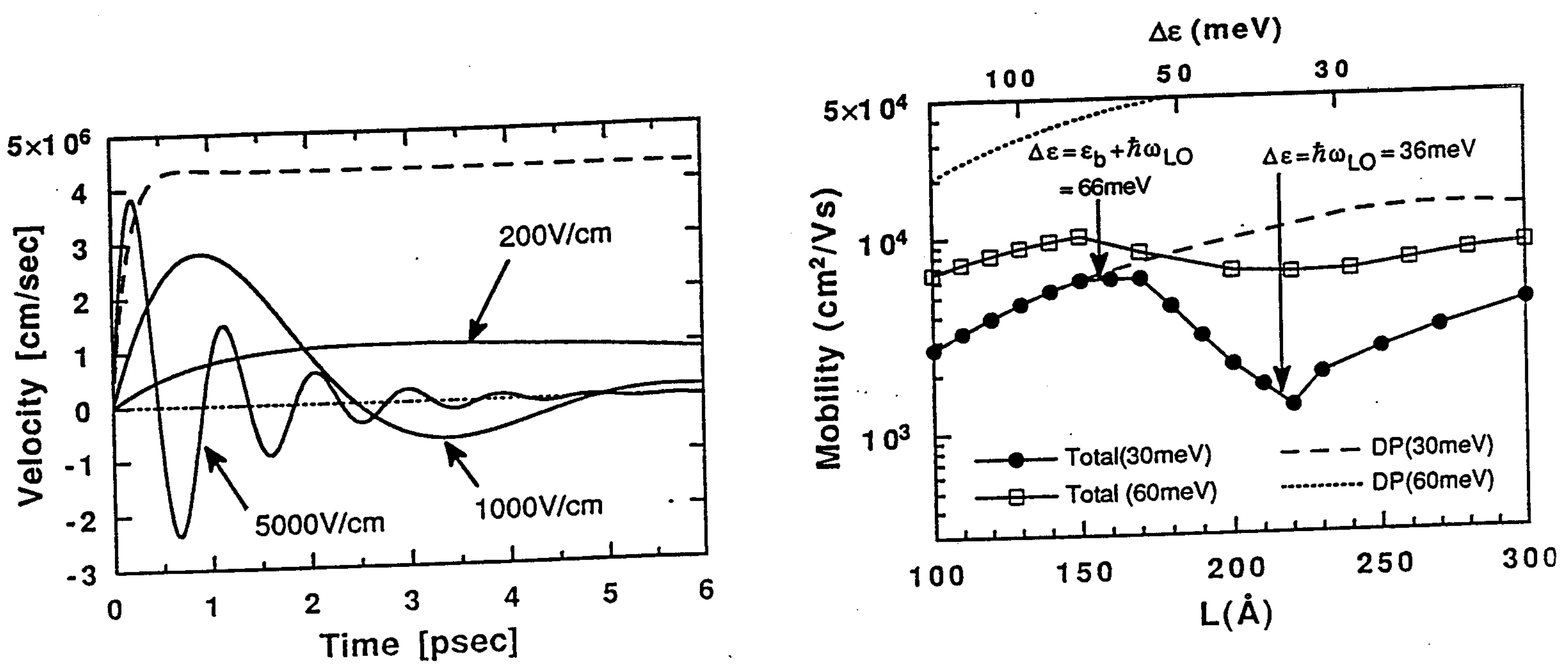

Fig. 2 (a). Electron velocity for three different electric fields (F = 200, 1000, and 5000V/cm) as functions of time at $T_L = 300K$ in a 1D-CQB. The solid lines are for a structure with (without) suppression of POP scattering. (b) Calculated mobility at $T_L = 300K$ as a function of the cross sectional width L of the wire. Square and solid circle denote the total mobility with and without pop scattering respectively. Dotted and dashed lines indicate the mobility determined by AP scattering.

Bloch oscillations with a period of a few picoseconds (Fig. 2.a). In steady-state analysis, we found that the carrier mobility is a strong function of the structure confinement and periodicity parameters (Fig.2.b).

The experimental simulation of 1D-CQB structures by using superlattices and high magnetic fields shows a plateau structure between the two resonances peaks that corresponds to suppression of optic phonon scattering. [P.3]

In the case of suppression of optic phonon scattering in 1D-CQB structures, we have also investigated the influence of umklapp process on acoustic phonon (AP) scattering rates [P.11]. A rigorous technique using imaginary time propagation has been used for modeling the electronic properties of the periodic systems. We found AP umklapp processes significant for intersubband scattering but negligible for intrasubband scattering.

II.3 Confined Phonon Scattering in Quantum Wires

We have calculated the total scattering rate in finite barrier GaAlAs-GaAs quantum wires based on the interaction Hamiltonian of confined longitudinal optic (LO) phonon and surface (SO) phonon modes [P.8]. With multisubband processes being properly taken into account our calculation indicates that for GaAs type of phonons the high frequency symmetric (s+) branch plays an important role among other SO phonon branches, and can even dominate over confined LO phonons in highly confined quantum wires as mentioned by Kim et al. (J. Appl. Phys. 70, 319 (1991)). Our results also demonstrate that the total contributions of confined LO and SO phonon scattering resemble closely to GaAs bulk phonon scattering. Selection rules between intersubband transition for SO modes suggest the possibility of a bottle-neck effect for carrier relaxation in square wires compared with rectangular wires.

Publications

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P.2. J. P. Leburton, "Non Equilibrium Carrier Statistics and Phonons Resonances in Quantum Wires," in Phonons in Semiconductor nanostructures, NATO ARW, Ed. J. P. Leburton, J. Pascual and C. Sotomayor-Torres, Kluwer Acad. Publisher, 1993, pp. 459-469.

P.3. H. Noguchi, T. Takamasu, N. Miura, J. P. Leburton and H. Sakaki, "Theoretical and Experimental Study of Electron Transport in One Dimensional Coupled Quantum Boxes," in Phonons in Semiconductor Nanostructures, NATO ARW, Ed. J. P. Leburton, J. Pascual and C. Sotomayor-Torres, Kluwer Acad. Publisher, 193, pp. 471-478.

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C.2. W. Jiang, J. P. Leburton and M. A. Stroscio, "Carrier Capture and Relaxation in 1D Rectangular Semiconductor Quantum Wires," March Meeting of the American Physical Society, March 16-20, 1992, Indianapolis, IN.

C.3. J. P. Leburton, "Non Equilibrium Carrier Statistics and Phonons Resonances in Quantum Wires," in Phonons in Semiconductor Nanostructures, NATO ARW, Ed. J. P. Leburton, J. Pascual and C. Sotomayor-Torres, Kluwer Acad. Publisher, 1993, pp. 459-469.

C.4. H. Noguchi, T. Takamasu, N. Miura, J. P. Leburton and H. Sakaki, "Theoretical and Experimental Study of Electron Transport in One Dimensional Coupled Quantum Boxes," in Phonons in Semiconductor Nanostructures, NATO ARW, Ed. J. P. Leburton, J. Pascual and C. Sotomayor-Torres, Kluwer Acad. Publisher, 193, pp. 471-478.

C.5. H. Noguchi, J. P. Leburton and H. Sakaki, "Electron Transport in One-Dimensional Coupled Quantum Boxes," Proceedings of the Symposium on GaAs and Related Compounds, Karuizawa, Japan, Sept. 28-Oct. 2, 1992, Inst. Phys. Conf. Ser. # 129, 299 (1992)

C.6. D. Jovanovic, T. Kawamura, J. P. Leburton, H. Chang, R. Grundbacher and I. Adesida, "Resonant Transport Phenomena in Thin-Gated Quasi-1D Systems," March Meeting of the American Physical Society, March 22-26, 1993, Seattle, WA.

C.7. T. Kawamura and J. P. Leburton, "Quantum Conductance of Double Bend Structures-Effect of Disorder," March Meeting of the American Physical Society, March 22-26, 1993, Seattle, WA.

C.8. J. Bigelow and J. P. Leburton, "Lateral Resonant Tunneling in Confined Heterostructures," 2nd International Sumposium on Quantum Confinement: Physics and Applications, 185th Meeting of the Electrochemical Society, San Francisco, CA., May 25-26, 1994.

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